Phenol, 3-methoxy-5-(2-phenylethyl)-
17635-59-5 | DTXSID80170114

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 78.6 °C

Global applicability domain: Inside

Local applicability domain index: 6.19e-01

Confidence level: 5.82e-01

Nearest Neighbors from the Training Set

Image not found
4-(Benzyloxyl)phenol
Measured: 122
Predicted: 95.1

Image not found
4-Phenoxyphenol
Measured: 84.0
Predicted: 87.2

Image not found
Ethanol, 2-(1-naphthalenyloxy)-
Measured: 45.0
Predicted: 69.9

Image not found
2-Propen-1-one, 1-(2-hydroxyphenyl)-3-phenyl-
Measured: 90.0
Predicted: 77.6

Image not found
2-Hydroxybenzophenone
Measured: 40.0
Predicted: 63.7